



chain nodes :

11	12	13	14	15	16	17	19	20	21	25	26	27	28	29	30	31	32	33	34	35	36	37	38	
39	40	41	48	49	50	61	62																	

ring nodes :

1	2	3	4	5	6	7	8	9	10	22	23	24	42	43	44	45	46	47						

chain bonds :

1-13	2-12	3-11	6-14	7-17	8-16	9-15	10-19	17-61	17-62	21-23	25-26	26-27	27-28											
27-29	30-31	31-38	32-33	33-34	34-39	35-37	36-40	40-41	42-48	48-49	49-50													

ring bonds :

1-2	1-6	2-3	3-4	4-5	4-7	5-6	5-10	7-8	8-9	9-10	22-23	22-24	23-24	42-43	42-47									
43-44	44-45	45-46	46-47																					

exact/norm bonds :

7-17	10-19	17-61	17-62	22-23	22-24	23-24	27-28	27-29															
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exact bonds :

1-13	2-12	3-11	6-14	8-16	9-15	21-23	25-26	26-27	30-31	31-38	32-33	33-34	34-39											
35-37	36-40	40-41	42-43	42-47	42-48	43-44	44-45	45-46	46-47	48-49	49-50													

normalized bonds :

1-2	1-6	2-3	3-4	4-5	4-7	5-6	5-10	7-8	8-9	9-10														
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isolated ring systems :

containing 42 :

G1:CN,NO2,X

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom	10:Atom	11:CLASS
12:CLASS	13:CLASS	14:CLASS	15:CLASS	16:CLASS	17:CLASS	19:CLASS	20:Atom	21:CLASS		
22:Atom	23:Atom	24:Atom	25:CLASS	26:CLASS	27:CLASS	28:CLASS	29:CLASS	30:CLASS	31:CLASS	
32:CLASS	33:CLASS	34:CLASS	35:CLASS	36:CLASS	37:CLASS	38:CLASS	39:CLASS	40:CLASS		
41:CLASS	42:Atom	43:Atom	44:Atom	45:Atom	46:Atom	47:Atom	48:CLASS	49:CLASS	50:CLASS	
61:CLASS	62:CLASS									

Generic attributes :

20:

Saturation : Saturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic